A Perturbation Analysis of the Problem of Downdating a Cholesky Factorization

C.-T. Pan
Department of Mathematical Sciences
Northern Illinois University
DeKalb, Illinois 60115

Submitted by Richard A. Brualdi

ABSTRACT

The rank-one modification of a Cholesky factorization $R^TR - \mathbf{z}\mathbf{z}^T = D^TD$, where R and D are upper triangular matrices and $\mathbf{z}$ is a column vector, is called the downdating problem. There are many articles devoted to this problem, due to its broad range of applications and numerical difficulty. This paper serves as a first-order parametrized perturbation analysis of this problem.

0. INTRODUCTION

The problem for finding the Cholesky factorization of

$$R^TR - \mathbf{z}\mathbf{z}^T,$$

where $R \in \mathbf{R}^{n\times n}$ is a real upper triangular matrix and $\mathbf{z} \in \mathbf{R}^n$ is a column vector (the lowercase boldface letters denote the vectors, the capital letters denote the matrices, and the superscript T means transpose), is called the *downdating problem* [18]. It is assumed here that $R^TR - \mathbf{z}\mathbf{z}^T$ is positive definite; the *downdated* Cholesky factor D then exists and satisfies

$$D^TD = R^TR - \mathbf{z}\mathbf{z}^T, \tag{1}$$

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where the upper triangular matrix D is unique up to the signs of the rows of D. The downdating problem has many important applications, such as modifying least-squares problems in signal processing [1, 13] and rank-one modification in quasi-Newton methods in optimization [8]. There are also several downdating algorithms available [3–5, 6, 9, 11, 12, 14–16, 18]. For the details of the algorithms and the numerical properties of these algorithms the reader is referred to these papers.

It has long been observed that, for the downdating problem, it is hard to compute the downdated Cholesky factor accurately on many occasions, or a breakdown may even occur during execution when the rounding error causes the problem to be indefinite. Stewart stressed in [17, 18] that the trouble we observe in computing the downdated Cholesky factor is not mainly caused by the algorithms but by the problem itself. In other words, the downdating problem (1) is a very sensitive problem; it is very easy for it to become ill conditioned, in which case no algorithm could give an accurate D.

From

$$R^T R - \mathbf{z}\mathbf{z}^T = R^T(I - \mathbf{a}\mathbf{a}^T)R = D^T D, \tag{2}$$

where $\mathbf{a}$ satisfies the linear system

$$R^T \mathbf{a} = \mathbf{z}, \tag{3}$$

it is easy to see that $R^T R - \mathbf{z}\mathbf{z}^T$ is positive definite if and only if $I - \mathbf{a}\mathbf{a}^T$ is positive definite. The only eigenvalue of $I - \mathbf{a}\mathbf{a}^T$ not equal to 1 is $1 - \|\mathbf{a}\|^2$ (where $\|\cdot\|$ denotes the Euclidean norm of a vector). Therefore, the necessary and sufficient condition for $R^T R - \mathbf{z}\mathbf{z}^T$ to be positive definite is $\|\mathbf{a}\| < 1$. Furthermore, Stewart [18] shows that the closeness of the Euclidean norm $\|\mathbf{a}\|$ to unity is a reliable signal for the corresponding downdating problem having trouble in computing an accurate downdated Cholesky factor.

Actually, if we assume that the Cholesky factorization $I - \mathbf{a}\mathbf{a}^T = A^T A$, we have $AR = D$. Consequently, $\|A^{-1}\| \leqslant \|R\|\,\|D^{-1}\|$, $\|R\| \leqslant \|A^{-1}\|\,\|D\|$, and $\|D^{-1}\| \leqslant \|R^{-1}\|\,\|A^{-1}\|$, where $\|\cdot\|$ is the spectral norm of a matrix. By invoking $\|A^{-1}\| = 1/\sqrt{1 - \|\mathbf{a}\|^2}$, the following inequalities are immediate:

$$\frac{\sigma_n}{\delta_n}, \frac{\sigma_1}{\delta_1} \leqslant \frac{1}{\sqrt{1 - \|\mathbf{a}\|^2}} \leqslant \frac{\sigma_1}{\delta_n}, \tag{4}$$

where $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_n$ are the singular values of R, and $\delta_1 \geqslant \delta_2 \geqslant \cdots \geqslant \delta_n$ are the singular values of D. From (4) we have

$$\sigma_n \leqslant \frac{\delta_n}{\sqrt{1 - \|\mathbf{a}\|^2}} \leqslant \sigma_1, \tag{5}$$

which means that the smallest singular value of D is always the same order of magnitude as the number $\sqrt{1 - \|\mathbf{a}\|^2}$, provided that the original upper triangular matrix R does not have widespread singular values, i.e., the condition number of R is not very large. Similar results can be found in [18] with a different approach.

However, the perturbation analysis performed in [18] is not a complete one, in the sense that it does not provide an upper bound for the *resulting error* (caused by perturbation error [19, xiii]). The information conveyed by the inequalities (4) and (5) does give us a reliable signal of the downdating problem being associated with an ill-conditioned $D^T D$, while $R^T R$ is well conditioned. However, the question of whether it also implies an ill-conditioned *downdating problem* remains unanswered.

Needless to say, *a priori* information on the condition number of the downdating problem is extremely important in both practice and theory. In this paper, we offer a solution to this long-standing problem. We shall give a first-order perturbation analysis of the downdating problem and then introduce the condition number of the problem.

The rest of this paper is organized as follows. Section 1 gives two lemmas. Section 2 presents the perturbation theorem. In Section 3, we discuss the possible choices of the condition number of the downdating problem in practice by selecting the dominant term in the perturbation bound.

1. PRELIMINARIES

In order to prove the main result we need several lemmas.

LEMMA 1.1. *Let*

$$I - \mathbf{a}\mathbf{a}^T = A^T A, \tag{6}$$

where $I \in \mathbf{R}^{n \times n}$ *is the identity matrix, and* $\mathbf{a} = (a_1, \dots, a_n)^T$ *is a vector with* $\|\mathbf{a}\| < 1$.

Then,

$$A = \begin{bmatrix} \frac{\beta_1}{\beta_0} & -\frac{a_1 a_2}{\beta_0 \beta_1} & -\frac{a_1 a_3}{\beta_0 \beta_1} & \cdots & -\frac{a_1 a_n}{\beta_0 \beta_1} \\ & \frac{\beta_2}{\beta_1} & -\frac{a_2 a_3}{\beta_1 \beta_2} & \cdots & -\frac{a_2 a_n}{\beta_1 \beta_2} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & \frac{\beta_n}{\beta_{n-1}} \end{bmatrix}, \tag{7}$$

where

$$\beta_k = \sqrt{1 - a_1^2 - a_2^2 - \cdots - a_k^2}, \qquad \beta_0 = 1. \tag{8}$$

Proof. The proof proceeds by direct verification. ∎

LEMMA 1.2. *Let* $\mathbf{a}(\epsilon)$ *be an entrywise differentiable function of* ϵ *defined on* $(-\alpha, \alpha) \subseteq \mathbf{R}$ *with* $\mathbf{a}(0) = \mathbf{a}$. *We also assume* $\|\mathbf{a}(\epsilon)\| < 1$ *for all* $\epsilon \in (-\alpha, \alpha)$. *Then the Cholesky factorization of*

$$I - \mathbf{a}(\epsilon)\mathbf{a}^T(\epsilon) = A^T(\epsilon) A(\epsilon)$$

exists, and $A(\epsilon)$ *is also entrywise differentiable (to the same order) for all* $\epsilon \in (-\alpha, \alpha)$. *Moreover, we have*

$$\sum_{k=1}^{n} \left| \frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)} \bigg|_{\epsilon=0} \right| \leqslant \frac{2\|\mathbf{a}\|}{\sqrt{1 - \|\mathbf{a}\|^2}} \left[\frac{\sqrt{n}\,\|\mathbf{a}\|^2}{\sqrt{1 - \|\mathbf{a}\|^2}} + 1 \right],$$

where $A_{ij}(\epsilon)$ *is the* (i, j) *entry of the matrix* $A(\epsilon)$, $a_k(\epsilon)$ *is the kth component of the vector* $\mathbf{a}(\epsilon)$, *and* $\partial A_{ij}(\epsilon)/\partial a_k(\epsilon)|_{\epsilon=0}$ *is the partial derivative of* $A_{ij}(\epsilon)$ *with respect to* $a_k(\epsilon)$ *evaluated at* $\epsilon = 0$.

Proof. From (7) we know

$$A_{ij}(\epsilon) = \begin{cases} \dfrac{\beta_i(\epsilon)}{\beta_{i-1}(\epsilon)}, & i = j, \\ -\dfrac{a_i(\epsilon)a_j(\epsilon)}{\beta_{i-1}(\epsilon)\beta_i(\epsilon)}, & i < j, \\ 0, & i > j, \end{cases} \tag{9}$$

where $\beta_i(\epsilon) = \sqrt{1 - a_1^2(\epsilon) - \cdots - a_i^2(\epsilon)}$, $\beta_0(\epsilon) = 1$. By using elementary calculus, it is easy to verify that

$$\left.\frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)}\right|_{\epsilon=0} = \begin{cases} -\dfrac{a_k a_i^2}{\beta_{i-1}^3 \beta_i}, & 1 \leqslant k \leqslant i-1, \\ -\dfrac{a_i}{\beta_{i-1}\beta_i}, & k = i, \\ 0, & k > i \end{cases} \qquad (\text{for} \quad i = j) \tag{10}$$

and

$$\left.\frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)}\right|_{\epsilon=0} = \begin{cases} -\dfrac{a_i a_j a_k(\beta_{i-1}^2 + \beta_i^2)}{\beta_{i-1}^3 \beta_i^3}, & 1 \leqslant k \leqslant i-1, \\ -\dfrac{a_j(\beta_i^2 + a_i^2)}{\beta_{i-1}\beta_i^3}, & k = i, \\ -\dfrac{a_i}{\beta_{i-1}\beta_i}, & k = j, \\ 0 & \text{otherwise} \end{cases} \qquad (\text{for} \quad i < j) \tag{11}$$

Hence, the value of $|\partial A_{ij}(\epsilon)/\partial a_k(\epsilon)|_{\epsilon=0}|$ only depends upon the absolute values of the components of $\mathbf{a}$. Instead of writing $|a_i|$, without loss of generality, we assume $a_i \geqslant 0$ for $1 \leqslant i \leqslant n$ as long as our only concern is the absolute value of (10) and (11). Thus we have

$$\sum_{k=1}^{n}\left|\frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)}\bigg|_{\epsilon=0}\right|$$

$$=\begin{cases}\dfrac{a_i}{\beta_{i-1}\beta_i}\left(\dfrac{a_i(a_1+\cdots+a_{i-1})}{\beta_{i-1}^2}+1\right), & i=j,\\[2ex] \dfrac{1}{\beta_{i-1}\beta_i}\left(\dfrac{a_ia_j(a_1+\cdots+a_{i-1})}{\beta_{i-1}^2}\right. \\[2ex] \qquad\left.+\dfrac{a_ia_j(a_1+\cdots+a_i)}{\beta_i^2}+a_i+a_j\right), & i<j,\end{cases} \tag{12}$$

where all a_i are assumed to be nonnegative now.

In order to estimate (12), we need the following inequalities, which are easy to verify:

$$\frac{a_i}{\beta_{i-1}} \leqslant \sqrt{a_1^2+\cdots+a_i^2} \leqslant \|\mathbf{a}\|, \tag{13}$$

and generally

$$\frac{a_j}{\beta_i} \leqslant \sqrt{a_1^2+\cdots+a_i^2+a_j^2} \leqslant \|\mathbf{a}\| \qquad \text{for} \quad i<j \tag{14}$$

and

$$\frac{1}{\beta_i} \leqslant \frac{1}{\beta_j} \leqslant \frac{1}{\sqrt{1-\|\mathbf{a}\|^2}} \qquad \text{for} \quad i \leqslant j. \tag{15}$$

Notice also that all the equalities in (13), (14), (15) are attainable for certain $\mathbf{a}$, i, and j.

Employing these inequalities, we have

$$\sum_{k=1}^{n} \left| \left. \frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)} \right|_{\epsilon=0} \right| \leqslant \begin{cases} \dfrac{\|\mathbf{a}\|^2}{\sqrt{1-\|\mathbf{a}\|^2}} \left(\dfrac{a_1 + \cdots + a_{i-1}}{\beta_{i-1}} + \dfrac{1}{\|\mathbf{a}\|} \right), & i = j, \\ \dfrac{2\|\mathbf{a}\|^2}{\sqrt{1-\|\mathbf{a}\|^2}} \left(\dfrac{a_1 + \cdots + a_i}{\beta_i} + \dfrac{1}{\|\mathbf{a}\|} \right), & i < j. \end{cases} \tag{16}$$

The following estimate is also attainable for some vector $\mathbf{a}$ and i (notice $a_i \geqslant 0$ are assumed):

$$\frac{a_1 + \cdots + a_{i-1}}{\beta_{i-1}} \leqslant \frac{a_1 + \cdots + a_i}{\beta_i} \leqslant \frac{\sqrt{n}\,\|\mathbf{a}\|}{\sqrt{1-\|\mathbf{a}\|^2}}. \tag{17}$$

Finally, we have

$$\begin{aligned} \sum_{k=1}^{n} \left| \left. \frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)} \right|_{\epsilon=0} \right| &\leqslant \frac{2\|\mathbf{a}\|^2}{\sqrt{1-\|\mathbf{a}\|^2}} \left(\frac{\sqrt{n}\,\|\mathbf{a}\|}{\sqrt{1-\|\mathbf{a}\|^2}} + \frac{1}{\|\mathbf{a}\|} \right) \\ &= \frac{2\|\mathbf{a}\|}{\sqrt{1-\|\mathbf{a}\|^2}} \left(\frac{\sqrt{n}\,\|\mathbf{a}\|^2}{\sqrt{1-\|\mathbf{a}\|^2}} + 1 \right). \qquad \blacksquare \end{aligned}$$

2. THE PERTURBATION ANALYSIS

In this section we state and prove the main results.

THEOREM 2.1. *Assume that the Cholesky factorization $R^T R - \mathbf{z}\mathbf{z}^T = D^T D$ exists, where R and D ($\in \mathbf{R}^{n \times n}$) are upper triangular, and $\mathbf{z}$ ($\in \mathbf{R}^n$) is a column vector. Let $\alpha > 0$ be small enough so that the Cholesky factorization*

$$D^T(\epsilon) D(\epsilon) = (R + \epsilon E)^T (R + \epsilon E) - (\mathbf{z} + \epsilon \mathbf{f})(\mathbf{z} + \epsilon \mathbf{f})^T, \tag{18}$$

always exists for $\epsilon \in (-\alpha, \alpha)$, where $\mathbf{f}$ is a given fixed column vector, and E is a given fixed upper triangular matrix.

Then, the resulting relative perturbation of $D(\epsilon)$ can be bounded as

$$\frac{\|D(\epsilon) - D\|}{\|D\|} \leqslant \kappa(R)\Bigg(\left[2n^{3/2}\kappa(R)C^2(\mathbf{a}) + 2n\kappa(R)C(\mathbf{a})\right]\frac{\|\mathbf{f}\|}{\|\mathbf{z}\|}|\epsilon|$$

$$+\left[2n^{3/2}\kappa(R)C^2(\mathbf{a}) + 2n\kappa(R)C(\mathbf{a}) + 1\right]\frac{\|E\|}{\|R\|}|\epsilon|\Bigg)$$

$$+O(\epsilon^2), \tag{19}$$

where

$$C(\mathbf{a}) = \frac{\|\mathbf{a}\|^2}{\sqrt{1 - \|\mathbf{a}\|^2}}, \tag{20}$$

and $\kappa(R) = \|R\|\,\|R^{-1}\|$ *is the condition number of the matrix* R.

Proof. Similarly to (2), we have

$$(R + \epsilon E)^T(R + \epsilon E) - (\mathbf{z} + \epsilon\mathbf{f})(\mathbf{z} + \epsilon\mathbf{f})^T$$

$$= (R + \epsilon E)^T\left[I - \mathbf{a}(\epsilon)\mathbf{a}^T(\epsilon)\right](R + \epsilon E), \tag{21}$$

where $\mathbf{a}(\epsilon)$ satisfies

$$(R + \epsilon E)^T\mathbf{a}(\epsilon) = \mathbf{z} + \epsilon\mathbf{f}. \tag{22}$$

Notice that each entry of the vector $\mathbf{a}(\epsilon)$ is a rational function of ϵ with the diagonal elements of $R + \epsilon E$ in its denominator, which are not zero. Thus, $\mathbf{a}(\epsilon)$ is entrywise differentiable. Since (21) is positive definite for $\epsilon \in (-\alpha, \alpha)$, we must have the Cholesky decomposition

$$I - \mathbf{a}(\epsilon)\mathbf{a}^T(\epsilon) = A(\epsilon)^T A(\epsilon), \tag{23}$$

where $\mathbf{a}(0) = \mathbf{a}$, $A(0) = A$, and

$$I - \mathbf{a}\mathbf{a}^T = A^T A. \tag{24}$$

Comparing (24) and (2), we have $D = AR$, where A has an explicit formula (7). Likewise, from (23) and (21) we have

$$D(\epsilon) = A(\epsilon)(R + \epsilon E), \tag{25}$$

where $A(\epsilon)$ has an explicit formula similar to (7).

Notice that

$$\|AR\|\,\|R^{-1}\| \geqslant \|A\| = 1, \quad \text{and} \quad \|A(\epsilon)\| = 1 \quad \text{on } (-\alpha, \alpha). \tag{26}$$

Therefore,

$$\begin{aligned}
\frac{\|D(\epsilon) - D\|}{\|D\|} &= \frac{\|A(\epsilon)(R + \epsilon E) - AR\|}{\|AR\|} \\
&= \frac{\|[A(\epsilon) - A]R + A(\epsilon)E\epsilon\|}{\|AR\|} \\
&\leqslant \frac{\|A(\epsilon) - A\|\|R\| + \|A(\epsilon)\|\|E\|\,|\epsilon|}{\|AR\|} \\
&\leqslant \|A(\epsilon) - A\|\|R\|\,\|R^{-1}\| + \|A(\epsilon)\|\|R^{-1}\|\,\|R\|\frac{\|E\|}{\|R\|}|\epsilon| \\
&= \kappa(R)\left[\|A(\epsilon) - A\| + \frac{\|E\|}{\|R\|}|\epsilon|\right].
\end{aligned} \tag{27}$$

Thus we must estimate $\|A(\epsilon) - A(0)\|$ for a small $\epsilon \in (-\alpha, \alpha)$. Invoking an inequality in [11, (2.6), p. 314], we have

$$\|A(\epsilon) - A(0)\| \leqslant n \max_{1 \leqslant i, j \leqslant n} |A_{ij}(\epsilon) - A_{ij}(0)| \tag{28}$$

However, according to Taylor's formula, we have

$$|A_{ij}(\epsilon) - A_{ij}(0)| \leqslant |A'_{ij}(0)||\epsilon| + O(\epsilon^2), \tag{29}$$

and

$$\max_{1\leqslant i,j\leqslant n}|A_{ij}(\epsilon)-A_{ij}(0)|\leqslant \max_{1\leqslant i,j\leqslant n}|A'_{ij}(0)||\epsilon|+O(\epsilon^2). \tag{30}$$

Now, if we consider $A_{ij}(\epsilon)=F(a_1(\epsilon),a_2(\epsilon),\dots,a_n(\epsilon))$ as a multivariable function of $a_1(\epsilon),\dots,a_n(\epsilon)$, it follows that

$$A'_{ij}(0)=\sum_{k=1}^{n}\left.\frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)}\right|_{\epsilon=0}a'_k(0),$$

and

$$\begin{aligned}|A'_{ij}(0)||\epsilon| &\leqslant \sum_{k=1}^{n}\left|\left.\frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)}\right|_{\epsilon=0}\right||a'_k(0)||\epsilon| \\ &\leqslant \sum_{k=1}^{n}\left|\left.\frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)}\right|_{\epsilon=0}\right||a_k(\epsilon)-a_k(0)|+O(\epsilon^2) \\ &\leqslant \|\mathbf{a}(\epsilon)-\mathbf{a}(0)\|\sum_{k=1}^{n}\left|\left.\frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)}\right|_{\epsilon=0}\right|+O(\epsilon^2). \end{aligned}\tag{31}$$

From (28) and (30), we have

$$\|A(\epsilon)-A\|\leqslant n\left(\max_{1\leqslant i,j\leqslant n}\sum_{k=1}^{n}\left|\left.\frac{\partial A_{ij}(\epsilon)}{\partial a_k(\epsilon)}\right|_{\epsilon=0}\right|\right)\|\mathbf{a}(\epsilon)-\mathbf{a}(0)\|+O(\epsilon^2). \tag{32}$$

From [10, p. 25] and (22) we have

$$\frac{\|\mathbf{a}(\epsilon)-\mathbf{a}\|}{\|\mathbf{a}\|}\leqslant\kappa(R)\left(\frac{\|\mathbf{f}\|}{\|\mathbf{z}\|}|\epsilon|+\frac{\|E\|}{\|R\|}|\epsilon|\right)+O(\epsilon^2). \tag{33}$$

Now the theorem is proved by substituting the results of Lemma 1.2 and (32) into (27). ■

3. THE CONDITION NUMBER OF THE DOWNDATING PROBLEM

From the bound of (19), we have the following conclusions:

1. The dominant term on the right-hand side of (19) is

$$h = \kappa^2(R)C^2(\mathbf{a}) \qquad \text{with} \quad C(\mathbf{a}) = \frac{\|\mathbf{a}\|^2}{\sqrt{1 - \|\mathbf{a}\|^2}}, \tag{34}$$

when $\|\mathbf{a}\|$ is close to 1. This is consonant with the observation made in [18] as well as the analysis derived from (4) and (5) in the Introduction. However, our perturbation analysis not only rigorously confirms that $1/\sqrt{1 - \|\mathbf{a}\|^2}$ is a decisive factor in signaling an ill-conditioned downdating problem, it also shows how the condition number of R itself affects the condition of the downdating problem.

2. The formula for $C(\mathbf{a})$ in (20) yields another important observation which has not been so clearly known. Notice that when $\|\mathbf{a}\|$ is small, the denominator $\|\mathbf{a}\|^2$ becomes the dominant factor of $C(\mathbf{a})$. This means that when the norm of $\mathbf{a}$ becomes relatively small, the condition of the downdating problem is improved much faster than just by the factor of $1/\sqrt{1 - \|\mathbf{a}\|}$ alone. In particular, when $\|\mathbf{a}\|$ is near zero, the condition number of the downdating problem is almost that of the original Cholesky factor R. This is also expected.

3. Our bound in (19) is very easy to compute if we use any condition estimator of a triangular matrix. For simplicity, we suggest using the following formula to assess the condition of the downdating problem:

$$\chi(\mathbf{a}, R) = \kappa(R)\left(1 + \frac{\kappa(R)\|\mathbf{a}\|^4}{1 - \|\mathbf{a}\|^2}\right). \tag{35}$$

4. The bound in (19) is very pessimistic when the perturbation is random. While we cannot show that for each R and $\mathbf{z}$ there always exist some particular perturbations in R and $\mathbf{z}$ such that the bound in (19) is attained, it is important to notice that in our proof of (19), each step of our estimation is attainable. In other words, this is the best bound we can get at present, even

if it is not the very best bound. The same philosophy used by Wilkinson [20, p. 170] for rounding-error analysis can be applied to the perturbation analysis here. As long as we know the roles that the different factors of the given problem play in contributing to the condition of the problem, we have reached our main purpose in the perturbation analysis.

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